

1-Hexadecanol
36653-82-4 | DTXSID4027991

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 16.5 days

Global applicability domain: Outside

Local applicability domain index: 3.82e-01

Confidence level: 8.91e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tetradecane</div> <div>Measured: 1370</div> <div>Predicted: 18.3</div>	<div>Image not found</div> <div>Tridecane</div> <div>Measured: 305</div> <div>Predicted: 13.5</div>	<div>Image not found</div> <div>Pentadecane</div> <div>Measured: 1810</div> <div>Predicted: 20.8</div>
<div>Image not found</div> <div>Dodecane</div> <div>Measured: 201</div> <div>Predicted: 10.6</div>	<div>Image not found</div> <div>Hexadecane</div> <div>Measured: 681</div> <div>Predicted: 20.1</div>	